

Magnetothermoelectric transport in modulated and unmodulated graphene

R. Nasir and K. Sabeeh[†]

Department of Physics, Quaid-i-Azam University, Islamabad 45320 Pakistan.

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Abstract

We draw motivation from recent experimental studies and present a comprehensive study of magnetothermoelectric transport in a graphene monolayer within the linear response regime. We employ the modified Kubo formalism developed for thermal transport in a magnetic field. Thermopower as well as thermal conductivity as a function of the gate voltage of a graphene monolayer in the presence of a magnetic field perpendicular to the graphene plane is determined for low magnetic fields (~ 1 Tesla) as well as high fields (~ 8 Tesla). We include the effects of screened charged impurities on thermal transport. We find good, qualitative as well as quantitative, agreement with recent experimental work on the subject. In addition, in order to analyze the effects of modulation, which can be induced by various means, on the thermal transport in graphene, we evaluate the thermal transport coefficients for a graphene monolayer subjected to a periodic electric modulation in a magnetic field. The results are presented as a function of the magnetic field and the gate voltage.

I. INTRODUCTION

Graphene exhibits remarkable thermal properties. The measured values of thermal conductivity of graphene reach as high as several thousand of watt per meter Kelvin[1–4], and these are among the highest values of known materials. Heat transport measures the energy carried by both electrons and phonons and is fundamental to understanding a material, its ground states, excitations and scattering mechanisms. If the dream of carbon-based electronics is to be realized, it is essential to study how and how fast heat is dissipated across graphene devices. This requires systematic measurements of thermal conductivity and thermopower over a broad temperature range (1.5-300 Kelvin) under various external conditions. Therefore, recently there has been considerable interest, both experimental[5–8] and theoretical[9–16], in the study of thermoelectric and magnetothermoelectric transport in graphene. This is partly due to the realization that the information provided by thermoelectric transport is complementary to electrical transport. And thermoelectric and magnetothermoelectric transport studies are extremely useful in providing insight on the scattering mechanism involved in transport. Fundamentally related to the electrical conductivity, the thermal conductivity and thermoelectric coefficients can be determined by the band structure and scattering mechanisms. The thermoelectric coefficients involve the energy derivatives of the electrical transport counterparts such as the conductivity σ [5]. Recent measurements of thermoelectric power (TEP) on graphene samples in zero and non-zero magnetic fields have shown a linear temperature dependence of TEP which suggest that the dominant contribution is that of diffusive thermopower (S_d). A comparison between the measured TEP and that predicted by the Mott formula shows general agreement, particularly at lower temperatures ($T < 50K$)[10]. However, at higher temperatures deviation from the Mott relation have been reported[6, 7]. In theoretical work, Yan et al.[15] have determined the TEP of Dirac fermions in graphene with in the self-consistent Born approximation. Also, Hwang et al.[9], in their calculation of TEP incorporate the energy dependence of various transport scattering rates and show that the dominant contribution is from the screened charged impurities in graphene’s environment. Further, Vaidya et al.[10] used Boltzmann transport theory to calculate S_d in graphene after considering contributions of optical phonon and surface roughness scatterings.

Application of a magnetic field in addition to a thermal gradient has profound effects on

the thermal transport in a system and serves as an additional probe. When a magnetic field is applied perpendicular to the $x-y$ plane of the sample, the diffusing charge carriers experience the Lorentz force. This results in developing a transverse electric field E_y in addition to the longitudinal field E_x . The thermopower is determined from the thermal gradient ∇T and the induced voltage ∇V as $S_{xx} = -\frac{\nabla V_x}{\nabla T}$ (also known as the Seebeck coefficient) and $S_{xy} = -\frac{\nabla V_y}{\nabla T}$ (the Nernst coefficient). They are a measure of the magnitude of the longitudinal and transverse voltages generated in response to an applied temperature gradient. They are very sensitive in graphene due to its semimetal nature[12]. The quantum magnetic oscillations in electrical and thermal transport have been earlier investigated theoretically by Gusynin and Sharapov[17] and they obtained analytical results for longitudinal thermal conductivity and the Nernst coefficient. However, they assumed a scattering rate that is constant in energy, independent of magnetic field and temperature. Hence the self energy used is not self consistent. Moreover, they evaluated the longitudinal thermal conductivity as a function of the magnetic field at different temperatures but at fixed chemical potential and constant impurity broadening. Further, they determined the Nernst coefficient (signal) without recourse to the modified Kubo formalism appropriate for thermal transport in a magnetic field. They neglected the dependence of Γ on the chemical potential/ carrier concentration. Dora and Thalmeier extended the work presented in [17] and studied the electric and thermal response of two dimensional Dirac fermions in a quantizing magnetic field in the presence of localized disorder[18]. They evaluated the Seebeck coefficient and the corresponding thermal conductivity as a function of the chemical potential and the magnetic field. They did not determine the Nernst coefficient and the transverse thermal conductivity.

What distinguishes our work on unmodulated graphene from the aforementioned previous papers is that we employ the modified Kubo formalism required to study thermal transport in a magnetic field. As has been discussed earlier, the usual Kubo formula for thermal response functions is invalid in a magnetic field and needs to be modified when calculating the transverse (Hall) thermal conductivity and the Nernst coefficient[19, 20]. We use the phenomenological transport equations obtained from the modified Kubo formalism[20, 21]. Further, in the scattering rate and the impurity broadening of the Landau levels the effects of the carrier concentration that can be varied by the gate voltage are taken into account. In the first stage, we determine the components of magnetoelectrothermal(MET) power and

MET conductivity of an unmodulated graphene monolayer in the presence of randomly distributed charged impurities. The results are presented as a function of the gate voltage for small and large magnetic fields applied perpendicular to the graphene sheet. We determine both the Nernst and Seebeck coefficients as well as longitudinal and transverse thermal conductivity. These results are then compared with experimental work. In addition, we have also carried out a detailed investigation of the MET transport properties of a graphene monolayer which is modulated by a weak one-dimensional periodic potential in the presence of a perpendicular magnetic field. Motivation for this has arisen from recent work, experimental and theoretical, that has shown that interaction with a substrate can lead to weak periodic modulation of the graphene spectrum. Furthermore, applying patterned gate voltage or placing graphene on a pre-patterned substrate can also lead to modulated graphene[22–24]. Placing impurities or adatom deposition can do the same. In a previous work, we have computed the electric transport coefficients of electrically modulated graphene[25]. It was shown that modulation turns the sharp Landau levels into bands whose width oscillates periodically with the magnetic field. This affects the magnetoelectric transport coefficients which exhibit commensurability (Weiss) oscillations. The origin of these Weiss oscillations is the commensurability of the two characteristic length scales of the system: The cyclotron diameter at the Fermi energy and the period of the modulation[26]. An interesting feature of electronic conduction in the modulated system is the opening of the diffusive (band) transport channel in addition to hopping (collisional) transport. Both these contributions to MET transport are taken into account in this work.

In the following section, we present the general formulation of the magnetoelectrothermal transport problem and perform the calculation of the thermopower and the thermal conductivity of unmodulated graphene as well as graphene subjected to one-dimensional (1D) weak periodic modulation. The results for the transport coefficients as a function of gate voltage (V_g) for unmodulated graphene are discussed in Section III, where we also make a comparison with experimental results. Following this in Section IV, the results for modulated graphene as a function of the gate voltage and the external magnetic field are presented. The present paper ends with a summary and conclusions.

II. THERMAL MAGNETOTRANSPORT COEFFICIENTS

As mentioned in the introduction, corrections to the usual Kubo formula for transport have to be made when studying thermal transport in a magnetic field. This was carried out by Luttinger, Smerka, Streda and Oji[20, 21]. We employ the modified Kubo formalism to determine the thermal transport coefficients from the electrical J_e and thermal (energy) current densities J_Q

$$J_{e\mu} = \mathcal{L}_{\mu\nu}^{(0)} \left[-\frac{1}{e} (\nabla_\nu \bar{\eta}) \right] + \frac{\mathcal{L}_{\mu\nu}^{(1)}}{e} \left[T \nabla_\nu \left(\frac{1}{T} \right) \right] \quad (1)$$

$$J_{Q\mu} = \frac{\mathcal{L}_{\mu\nu}^{(1)}}{e} \left[-\frac{1}{e} (\nabla_\nu \bar{\eta}) \right] + \frac{\mathcal{L}_{\mu\nu}^{(2)}}{e^2} \left[T \nabla_\nu \left(\frac{1}{T} \right) \right]. \quad (2)$$

Here $\bar{\eta} = \eta - e\phi$ with η the chemical potential, ϕ the scalar potential, e the electronic charge and T the temperature of the system. The electrical and thermal transport coefficients: the electrical conductivity σ , thermopower S and the thermal conductivity κ can be obtained from the above expressions, following [20, 21, 27–29], as

$$\sigma_{\mu\nu} = \mathcal{L}_{\mu\nu}^{(0)}, \quad (3)$$

$$S_{\mu\nu} = \frac{1}{eT} [(\mathcal{L}^{(0)})^{-1} \mathcal{L}^{(1)}]_{\mu\nu}, \quad (4)$$

$$\kappa_{\mu\nu} = \frac{1}{e^2 T} [\mathcal{L}_{\mu\nu}^{(2)} - eT (\mathcal{L}^{(1)} S)_{\mu\nu}] \quad (5)$$

with

$$\mathcal{L}_{\mu\nu}^{(\alpha)} = \int dE \left[-\frac{\partial f(E)}{\partial E} \right] (E - \eta)^\alpha \sigma_{\mu\nu}(E). \quad (6)$$

$\mathcal{L}_{\mu\nu}^{(\alpha)}$ ($\alpha = 0, 1, 2$) are, in general, tensors where $\mu, \nu = x, y$. These phenomenological transport coefficients satisfy the Onsager relation [21, 27] $\mathcal{L}_{\mu\nu}^{(\alpha)}(B) = \mathcal{L}_{\nu\mu}^{(\alpha)}(-B)$. $\sigma_{\mu\nu}(E)$ is the zero-temperature conductivity and $f(E) = [\exp(\frac{E-\eta}{k_B T}) + 1]^{-1}$ is the Fermi Dirac distribution function with η the chemical potential. The quantity $\rho_{\mu\nu} = (\mathcal{L}^{(0)})_{\mu\nu}^{-1}$ is the resistivity tensor whose components are $\rho_{xx} = \sigma_{yy}/\Lambda$, $\rho_{yy} = \sigma_{xx}/\Lambda$, $\rho_{xy} = -\rho_{yx} = \sigma_{yx}/\Lambda$ with $\Lambda = \sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}$.

In order to calculate the thermal transport coefficients for graphene, we consider a graphene monolayer in the xy -plane subjected to a magnetic field B along the z -direction. In the Landau gauge, the unperturbed single particle Dirac-like Hamiltonian may be written as

$$H_o = v_F \sigma \cdot (-i\hbar \nabla + e\mathbf{A}). \quad (7)$$

Here, $\sigma = \{\sigma_x, \sigma_y\}$ are the Pauli matrices and $v_F = 10^6 \text{ m/s}$ characterizes the electron velocity with $\mathbf{A} = (0, Bx, 0)$ the vector potential. The normalized eigenfunctions of the Hamiltonian given in Eq.(7) are

$$\Psi_{n,k_y} = \frac{e^{ik_y y}}{\sqrt{2L_y l}} \begin{pmatrix} -i\phi_{n-1}[(x+x_o)/l] \\ \phi_n[(x+x_o)/l] \end{pmatrix}, \quad (8)$$

where $\phi_n(x)$ and $\phi_{n-1}(x)$ are the harmonic oscillator wavefunctions centred at $x_o = l^2 k_y$. n is the Landau level index, $l = \sqrt{\frac{\hbar}{eB}}$ the magnetic length and L_y the length of 2D graphene system in the y -direction. The corresponding eigenvalue is $E_n = \hbar\omega_g \sqrt{n}$ where $\omega_g = v_F \sqrt{2eB/\hbar} = v_F \sqrt{2}/l$ is the cyclotron frequency of the Dirac electrons in graphene.

In order to investigate the effects of modulation, we express the Hamiltonian in the presence of modulation as $H = H_o + U(x)$. Here, $U(x)$ is the one-dimensional periodic modulation potential along the x -axis. It is given by $U(x) = V_e \cos Kx$ such that $K = \frac{2\pi}{a}$, a is the period of modulation and V_e is the constant modulation amplitude. To account for weak modulation, we take V_e to be an order of magnitude smaller than the Fermi energy $E_F = v_F \hbar k_F$, where $k_F = \sqrt{2\pi n_e}$ is the magnitude of Fermi wave vector with n_e the density of electrons. This allows us to apply standard first order perturbation theory to determine the energy eigenvalues in the presence of modulation. Thus, energy eigenvalues for weak modulation ($V_e \ll E_F$), are $E_{n,k_y} = E_n + F_{n,B} \cos Kx$. Here, $F_{n,B} = \frac{V_e}{2} \exp(-\frac{u}{2}) [L_n(u) + L_{n-1}(u)]$, $u = \frac{K^2 l^2}{2}$ and, $L_n(u)$ and $L_{n-1}(u)$ are Laguerre polynomials.

In the presence of a periodic modulation, there are two contributions to magnetoconductivity: the collisional (hopping) contribution and the diffusive (band) contribution. The former is the localized state contribution which carries the effects of Shubnikov de Hass (SdH) oscillations that are modified by periodic modulation. The diffusive contribution is the extended state contribution and arises due to finite drift velocity acquired by the charge carriers in the presence of modulation. In the linear response regime, the conductivity tensor is a sum of a diagonal and a non diagonal part : $\sigma_{\mu\nu}(\omega) = \sigma_{\mu\nu}^d(\omega) + \sigma_{\mu\nu}^{nd}(\omega)$, $\mu, \nu = x, y$. In general, $\sigma_{\mu\nu}^d(\omega) = \sigma_{\mu\nu}^{diff}(\omega) + \sigma_{\mu\nu}^{col}(\omega)$, accounting for both diffusive and collisional contribution whereas $\sigma_{\mu\nu}^{nd}(\omega)$ is the Hall contribution. Here, $\sigma_{xx} = \sigma_{xx}^{col}$ and $\sigma_{yy} = \sigma_{xx}^{col} + \sigma_{yy}^{diff}$. Similar to the conductivity tensors, the diagonal components of the thermal transport coefficients are determined by the following expressions:

$$\mathcal{L}_{xx}^{(\alpha)} = \mathcal{L}_{xx}^{(\alpha) col} = \mathcal{L}_{yy}^{(\alpha) col} \quad (9)$$

$$\mathcal{L}_{yy}^{(\alpha)} = \mathcal{L}_{yy}^{(\alpha)diff} + \mathcal{L}_{yy}^{(\alpha)col}. \quad (10)$$

The finite temperature conductivity components $\sigma_{\mu\nu}$ have been evaluated in [25] for scattering by random screened charged impurities of density N_I with impurity broadening Γ . The screened potential (in Fourier space) is $U_o = 2\pi e^2/\epsilon\sqrt{q^2 + k_s^2}$, which is valid for small wave vectors, $q \ll k_s$, k_s being the inverse screening length and ϵ the dielectric constant. Therefore, from Eq.(6), we obtain the zero-temperature phenomenological transport coefficients $\mathcal{L}_{\mu\nu}^{(\alpha)}$ as

$$\mathcal{L}_{yy}^{(\alpha)diff} = 2\frac{e^2}{h}\frac{\tau}{\hbar}u\sum_{n=0}^{\infty}[F_{n,B}]^2[E-\eta]^\alpha\left[\frac{-\partial f(E)}{\partial E}\right]_{E=E_n}, \quad (11)$$

$$\mathcal{L}_{xx}^{(\alpha)col} \approx \frac{e^2}{h}\frac{\beta N_I U_o^2}{\pi a \Gamma}\sum_{n=0}^{\infty}n\int_0^{a/l^2}dk_y[E-\eta]^\alpha f_{n,k_y}(1-f_{n,k_y}), \quad (12)$$

and

$$\mathcal{L}_{yx}^{(\alpha)} = \frac{e^2}{h}\frac{l^2}{a}\sum_{n=0}^{\infty}\int_0^{a/l^2}dk_y\frac{1}{[(E_{n+1,k_y}-E_{n,k_y})/\hbar\omega_g]^2}\int_{E_{n,k_y}}^{E_{n+1,k_y}}dE\left\{[E-\eta]^\alpha\left[\frac{-\partial f(E)}{\partial E}\right]\right\}_{E_{n,k_y}}, \quad (13)$$

where τ is the scattering time. Here, we have taken the scattering time to be independent of Landau-level index n . And the components of thermopower are given by the following equations:

$$S_{xx} = \frac{1}{eT}\left[\left(\frac{\sigma_{yy}}{S_o}\right)\mathcal{L}_{xx}^{(1)} + \left(\frac{1}{\sigma_{yx}}\right)\mathcal{L}_{yx}^{(1)}\right], \quad (14)$$

$$S_{yy} = \frac{1}{eT}\left[\left(\frac{\sigma_{xx}}{S_o}\right)\mathcal{L}_{yy}^{(1)} + \left(\frac{1}{\sigma_{yx}}\right)\mathcal{L}_{yx}^{(1)}\right] \quad (15)$$

and

$$S_{xy} = \frac{1}{eT}\left[\left(\frac{\sigma_{yy}}{S_o}\right)(-\mathcal{L}_{yx}^{(1)}) + \left(\frac{1}{\sigma_{yx}}\right)\mathcal{L}_{yy}^{(1)}\right], \quad (16)$$

$$S_{yx} = \frac{1}{eT}\left[\left(\frac{\sigma_{xx}}{S_o}\right)\mathcal{L}_{yx}^{(1)} + \left(-\frac{1}{\sigma_{yx}}\right)\mathcal{L}_{xx}^{(1)}\right]. \quad (17)$$

The components of the thermal conductivity are given by

$$\kappa_{xx} = \frac{1}{e^2T}\left[\mathcal{L}_{xx}^{(2)} - eT\left\{\mathcal{L}_{xx}^{(1)}S_{xx} - \mathcal{L}_{yx}^{(1)}S_{yx}\right\}\right], \quad (18)$$

$$\kappa_{yy} = \frac{1}{e^2T}\left[\mathcal{L}_{yy}^{(2)} - eT\left\{\mathcal{L}_{yx}^{(1)}S_{xy} + \mathcal{L}_{yy}^{(1)}S_{yy}\right\}\right] \quad (19)$$

and

$$\kappa_{xy} = \frac{1}{e^2T}\left[-\mathcal{L}_{yx}^{(2)} - eT\left\{\mathcal{L}_{xx}^{(1)}S_{xy} - \mathcal{L}_{yx}^{(1)}S_{yy}\right\}\right], \quad (20)$$

$$\kappa_{yx} = \frac{1}{e^2T}\left[\mathcal{L}_{yx}^{(2)} - eT\left\{\mathcal{L}_{yx}^{(1)}S_{xx} + \mathcal{L}_{yy}^{(1)}S_{yx}\right\}\right]. \quad (21)$$

III. MAGNETOTHERMOPOWER AND MAGNETOTHERMAL CONDUCTIVITY OF UNMODULATED GRAPHENE

From the electrical conductivity $\sigma_{\mu\nu}$, calculated in our previous work [25], we determine the phenomenological transport coefficients $\mathcal{L}_{yx}^{(\alpha)}$ employing Eqs.11, 12 and 13. Employing these, the components of thermopower and thermal conductivity are numerically evaluated using Eqs.14 through 21. The results for the magnetoelectrothermal transport properties of an unmodulated graphene monolayer as a function of the gate voltage are presented in this section. The number density n_e is related to the gate voltage V_g through the relationship $n_e = \epsilon_o \epsilon V_g / te$, where ϵ_o and $\epsilon = 3.9$ are the permittivities for free space and the dielectric constant for graphene on a SiO_2 substrate, respectively. The electron charge is e and $t(\approx 300\text{nm})$ is the thickness of the sample [30]. The components of thermopower ($S_{\mu\nu}$) and thermal conductivity ($\kappa_{\mu\nu}$), as the system moves away from the charge neutral point on the electron side on changing the gate voltage, are shown in Fig. (1) at a magnetic field of one Tesla. The lattice temperature of 10K and mobility of $\mu = 20\text{m}^2/\text{Vs}$ [31] is chosen. The scattering time is related to the mobility as $\tau = \frac{\mu E_F}{ev_F^2}$ in a graphene monolayer[32]. Since impurity broadening Γ can be expressed in terms of the self energy $\Sigma^-(E)$ as $\Gamma \equiv \Gamma(E) = 2 \text{Im} [\Sigma^-(E)]$ and also $\Gamma(E) = \hbar/\tau$ [33]. We use the expression for $\text{Im} [\Sigma^-(E)]$ derived in [25] to find $\Gamma = \sqrt{\hbar(\hbar\omega_g)^2/(4\pi\tau E_F)}$. The electron number density is $n_e = 7.19V_g \times 10^{14}\text{m}^{-2}$ and Fermi energy is $E_F = \hbar v_F \sqrt{2\pi n_e} = 44.3\sqrt{V_g}\text{meV}$. And the impurity density is related to Γ through $N_I = \pi l^2 \Gamma^2 / U_o^2$ [34]. The scattering time of $\tau = 4.431\mu\sqrt{V_g} \times 10^{-14}\text{s}$, impurity broadening $\Gamma = 5.934\sqrt{B/(\mu V_g)}\text{meV}$ and impurity density $N_I = \frac{2.46}{\mu} \times 10^{14}\text{m}^{-2}$ were employed in this work[31–37]. Moreover, the same study is carried out at a higher magnetic field of 8.8T for graphene with mobilities of $\mu = 1\text{m}^2/\text{Vs}$ and $\mu = 20\text{m}^2/\text{Vs}$ respectively and the results are shown in Fig. (2). Since S_{xx} and S_{yy} are identical so only S_{xx} is depicted in these figures. The longitudinal coefficient of thermopower (S_{xx}) is equivalent to the Seebeck coefficient and our results provide a qualitative as well as quantitative understanding of the overall behavior of the observed $S_{xx}(V_g)$. S_{xx} can have either sign and it is negative in our case since the charge carriers are electrons in this range of V_g . The transverse component of thermopower (S_{yx}) is also known as the Nernst signal and it arises due to the presence of the perpendicular magnetic field as the Lorentz force bends the trajectories of the thermally diffusing carriers. It can be seen from Fig. (1a) and Fig. (2a) that S_{xx} follows $1/\sqrt{V_g}$ (with

$V_g \propto n_e$). Similar behavior of S_{xx} is observed in experiments[5–7]. Notice that we have presented results for diffusive thermopower and we have ignored the phonon contribution to thermopower due to weak electron phonon coupling in graphene [6, 9]. S_{xx} and S_{yx} ($S_{yx} = -S_{xy}$) both show Shubnikov-de Haas (SdH) type oscillations in the Landau quantizing magnetic field. At the lower magnetic field of 1 Tesla (Fig. (1)), the oscillations are more closely spaced since the separation between the Landau levels, which is proportional to the magnetic field strength, is smaller compared to the results for the higher magnetic field of 8.8 Tesla, (Fig. (2)). Moreover, we observe in Figs. (1a) and (2a) that both S_{xx} and S_{yx} approach zero at those values of V_g where there are boundaries of Landau Levels and no carriers are available to participate in transport. The peaks of S_{xx} are observed at the centre of Landau levels. With the increase in V_g and hence an increase in n_e , higher Landau levels are occupied. The oscillations in S_{xx} and S_{xy} are damped as we increase V_g . The reason for this is that higher V_g corresponds to higher values of the Fermi energy and if the Fermi energy is much larger than the Landau level separation, Landau quantization effects are lost. At $B = 8.8T$, (Fig. (2a)), the oscillations in S_{xx} and S_{xy} show that the width of the peaks broaden compared to those for smaller magnetic field of $B = 1T$. At lower magnetic field, the separation between the Landau levels is smaller compared to higher fields with the result that the peaks of S_{xx} are more closely spaced. Furthermore, the overall magnitude of S_{xx} and S_{xy} increases with increasing magnetic field strength (See Fig. 1a and Fig. 2a). In these figures, we also present thermal conductivity as a function of the gate voltage. The longitudinal thermal conductivity κ_{xx} shows oscillating behavior which damps out as V_g increases, where Landau quantization effects become less significant. However, the transverse component of thermal conductivity κ_{yx} rises monotonically with V_g as shown in Fig. (1b) and Fig. (2b). At the higher magnetic field, quantum Hall steps have begun to appear. The behavior of longitudinal and transverse thermal conductivity follows that of the corresponding components of electrical conductivity. At higher magnetic fields, the splitting of the peaks in the longitudinal thermal conductivity κ_{xx} is seen in Fig. (2b) which was also observed in [18] where it is shown that the splitting occurs in such a way that they produce antiphase oscillations with respect to the electric one and lead to the violation of the Wiedemann-Franz law. For the un-modulated case, $\sigma_{yy} = \sigma_{xx}$, $\mathcal{L}_{xx}^{(\alpha)} = \mathcal{L}_{yy}^{(\alpha)}$ and using Eq.(14) through Eq.(21) we find that $S_{yx} = -S_{xy}$, $\kappa_{xx} = \kappa_{yy}$ and $\kappa_{xy} = -\kappa_{yx}$. Therefore, only κ_{xx} and κ_{yx} are shown in the figures. We find that the results for magnetothermal

power obtained in our work at $B = 8.8T$ with $T = 10K$ are in good agreement, both qualitative and quantitative, with the experimental results obtained in [6, 7], see Fig (3) of [6]. These results do indicate that scattering from screened charged impurities is the dominant scattering mechanism required to explain the experimental results. We must add that our quantitative results for S_{yx} depend strongly on the mobility of the graphene system.

IV. MAGNETOTHERMOPOWER AND MAGNETOTHERMAL CONDUCTIVITY OF PERIODICALLY MODULATED GRAPHENE

Now we consider the effects of modulation. The 1D modulation broadens the sharp Landau levels into bands and gives rise to an additional diffusive (or band) contribution to transport. This additional contribution is absent without modulation. We now focus on the modulation induced changes in the thermal magnetotransport coefficients of graphene. Therefore, in the first part we present the thermopower and thermal conductivity of modulated graphene with mobility of $20m^2/Vs$ as a function of the gate voltage. These are shown in Fig. (3) and Fig. (5) respectively. The results are for a constant external magnetic field of $B = 1T$ applied perpendicular to the graphene sheet, with electric modulation of strength $V_e = 3meV$ applied in the x -direction at a temperature of $T = 10K$. In this case $\Gamma = \frac{1.3}{\sqrt{V_g}}meV$ and $\hbar\omega_g = 36.3meV$, such that $\Gamma \ll V_e \ll \hbar\omega_g$ to satisfy the requirements of weak modulation. The period of modulation is $a = 382nm$. The results for S_{xx} and S_{yy} are identical, so only S_{xx} is shown in these figures. The amplitude of oscillations in S_{xx} (ΔS_{xx}) is greater than that of S_{xy} (ΔS_{xy}) which damps out with increasing gate voltage(V_g). Both S_{xx} and S_{xy} show SdH-type oscillations and it verifies that the system is Landau quantized. The modulation effects are apparent in S_{xx} and S_{xy} which shows modulation of SdH-type oscillations and $\Delta S_{xx} \gg \Delta S_{xy}$, Fig. (3). κ_{yx} is greater than κ_{xx} and κ_{yy} as shown in Fig. (5). These modulation induced effects on thermal transport coefficients can be highlighted by calculating the difference between the modulated case and the un-modulated case. The contribution of modulation to thermopower $\Delta S_{\mu\nu}(V_e) = \Delta S_{\mu\nu}(V_e) - \Delta S_{\mu\nu}(0)$ and thermal conductivity $\Delta\kappa_{\mu\nu}(V_g) = \Delta\kappa_{\mu\nu}(V_e) - \Delta\kappa_{\mu\nu}(0)$ are shown in Fig. (4) and Fig. (6) respectively. These figures clearly show the modulation of SdH oscillations in both the thermopower and the thermal conductivity. For an un-modulated case $\kappa_{xx} = \kappa_{yy}$, however for modulated graphene $\kappa_{xx} \neq \kappa_{yy}$ and this expected behaviour is seen in Fig. (6) where $\Delta\kappa_{xx} \neq \Delta\kappa_{yy}$.

The 1D modulation gives a positive contribution to $\Delta\kappa_{yy}$ while $\Delta\kappa_{xx}$ and $\Delta\kappa_{yx}$ oscillate around zero. $\Delta\kappa_{yy} \gg \Delta\kappa_{xx}$, which is a consequence of the fact that $\Delta\kappa_{xx}$ has only collisional contribution, whereas $\Delta\kappa_{yy}$ in addition to the collisional part, has large contribution from band conduction.

We also show the results when the magnetic field is varied and the electron density is fixed at $n_e = 3.16 \times 10^{15} m^{-2}$ which corresponds to a gate voltage of $V_g = 4.39V$. The Fermi energy of the system is $E_F = \hbar v_F \sqrt{2\pi n_e} \approx 92.3 meV$. We have taken the mobility of $20 m^2/Vs$ [31] and hence scattering time is taken to be $\tau = 1.86 \times 10^{-12} s$. Impurity broadening $\Gamma = 0.633\sqrt{B} meV$ and impurity density $N_I = 1.23 \times 10^{13} m^{-2}$ were employed in this part of the work. The strength of the electrical modulation is taken to be $V_e = 2 meV$ with period $a = 382 nm$ and temperature $T = 10 K$. The difference between the modulated case and the unmodulated case highlights the modulation induced effects in these thermoelectric quantities. The thermopower and the change in thermopower due to modulation $\Delta S_{\mu\nu}(B)$ are shown in Fig. (7) as a function of the magnetic field in the units of $-k_B/e$. When B is less than $0.2T$ Weiss oscillations are observed whereas SdH type oscillations dominate at higher magnetic fields. It is also seen that these oscillations in S_{xx} are 90° out of phase with those in S_{xy} . The amplitude of the oscillations in $\Delta S_{xx} \gg \Delta S_{xy}$ and they are 90° out of phase. Again for B greater than $0.2T$ the oscillations appear as envelopes of SdH oscillations. The different components of the thermal conductivity tensor and the correction to it due to 1D modulation are shown in Fig. (8). The magnetic field dependence of the thermal conductivity tensor is similar to that of the electrical conductivity tensor obtained in [25]. In Fig. (8) we see that $\Delta\kappa_{yx} \gg \Delta\kappa_{yy} \gg \Delta\kappa_{xx}$, such that $\Delta\kappa_{yx}$ and $\Delta\kappa_{xx}$ are 180° out of phase from each other.

To conclude, in this work we have studied magnetothermoelectric transport in graphene in the linear response regime using the modified Kubo formalism appropriate for thermal transport in a magnetic field. Results are presented for both unmodulated graphene as well as graphene that is weakly modulated by an electric modulation. We take into account scattering from screened charged impurities and our results indicate that these provide the most dominant scattering mechanism at low temperatures. The thermopower, the Seebeck coefficient and the Nernst coefficient are determined as a function of the gate voltage. Furthermore, we also determine the magnetothermal conductivity tensor, both the longitudinal and the transverse (Hall) components. For unmodulated graphene we were able to make a

comparison of the thermopower with experimental results and find that they are in good agreement, both qualitative as well as quantitative, with experimental results. In the case of modulated graphene, we focus on the modulation induced effects that appear as commensurability (Weiss-type) oscillations in the magnetothermoelectric coefficients. The results are presented as both functions of the gate voltage and the magnetic field.

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† Corresponding author: ksabeeh@qau.edu.pk

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